ELSEVIER

5 August 1994

Chemical Physics Letters 225 (1994) 548–556

CHEMICAL PHYSICS LETTERS

Author index to volume 225

Adamowicz, L., see G.H. Roehrig 225 (1994) 265
Ageev, S.Z. and B.C. Sanctuary, Shaped pulses in NQR 225 (1994) 499
Agreiter, J., A.M. Smith, M. Härtle and V.E. Bondybey, Laser-induced fluorescence of matrix-isolated $C_4N_2^+$ 225 (1994) 87
Allan, M., Measurement of absolute differential cross section for the excitation of the lowest triplet state of ethene 225 (1994) 156
Amstrup, B. and S.A. Rice, Optimal control theory approach to enhancement of HgAr photodissociation 225 (1994) 1
Ángyán, J.G., see P. Surján 225 (1994) 258
Antoine, R., see Ph. Dugourd 225 (1994) 28
Ayala, P.Y. and H.B. Schlegel, An ab initio molecular orbital study of $SiH_2+F_2 \rightarrow SiH_2F_2$ 225 (1994) 410

Bajdor, K., see A.M. Brouwer 225 (1994) 386
Baldus, M., see M. Tomaselli 225 (1994) 131
Barron, L.D., see L. Hecht 225 (1994) 519, 525
Bartlett, R.J., see H. Sekino 225 (1994) 486
Basché, Th., S. Kummer and C. Bräuchle, Optical spectroscopy of single pentacene molecules in an ordered and a disordered *p*-terphenyl crystal 225 (1994) 116
Bässler, H., see M. Scheidler 225 (1994) 431
Bates, S. and J. Dwyer, Improvements in ab initio calculated OH stretching frequencies of zeolite acid site models and other OH-containing molecules, using a Morse potential 225 (1994) 427
Bauschlicher Jr., C.W., see J.A. Sheehy 225 (1994) 221
Bauschlicher Jr., C.W., see P. Maitre 225 (1994) 467
Bishop, A.R., see S.P. Love 225 (1994) 170
Bondarev, S.L. and V.N. Knyukshto, Fluorescence from the $S_1(2^1A_g)$ state of all-trans-β-carotene 225 (1994) 346
Bondybey, V.E., see J. Agreiter 225 (1994) 87
Botschwina, P., Large-scale ab initio calculations of spectroscopic constants for CNCN 225 (1994) 480
Bräuchle, C., see Th. Basché 225 (1994) 116
Braun, D., A. Ceulemans, B. Dick and H. Konami, Spectral hole burning on silicon phthalocyanines isolated in an argon matrix 225 (1994) 398
Brousseau, J.-L., see C. Garrigou-Lagrange 225 (1994) 297
Brouwer, A.M., F.W. Langkilde, K. Bajdor and R. Wilbrandt, Through-bond interaction in the radical cation of N,N-dimethylpiperazine. Resonance Raman spectroscopy and quantum chemical calculations 225 (1994) 386
Broyer, M., see Ph. Dugourd 225 (1994) 28
Bürgi, T., T. Droz and S. Leutwyler, Ground-state binding energy and vibrations of the carbazole·Ar van der Waals complex by pump/dump-R2PI measurements 225 (1994) 351

ELSEVIER

5 August 1994

Chemical Physics Letters 225 (1994) 548–556

CHEMICAL PHYSICS LETTERS

Author index to volume 225

Adamowicz, L., see G.H. Roehrig 225 (1994) 265
Ageev, S.Z. and B.C. Sanctuary, Shaped pulses in NQR 225 (1994) 499
Agreiter, J., A.M. Smith, M. Härtle and V.E. Bondybey, Laser-induced fluorescence of matrix-isolated $C_4N_2^+$ 225 (1994) 87
Allan, M., Measurement of absolute differential cross section for the excitation of the lowest triplet state of ethene 225 (1994) 156
Amstrup, B. and S.A. Rice, Optimal control theory approach to enhancement of HgAr photodissociation 225 (1994) 1
Ángyán, J.G., see P. Surján 225 (1994) 258
Antoine, R., see Ph. Dugourd 225 (1994) 28
Ayala, P.Y. and H.B. Schlegel, An ab initio molecular orbital study of $SiH_2+F_2 \rightarrow SiH_2F_2$ 225 (1994) 410

Bajdor, K., see A.M. Brouwer 225 (1994) 386
Baldus, M., see M. Tomaselli 225 (1994) 131
Barron, L.D., see L. Hecht 225 (1994) 519, 525
Bartlett, R.J., see H. Sekino 225 (1994) 486
Basché, Th., S. Kummer and C. Bräuchle, Optical spectroscopy of single pentacene molecules in an ordered and a disordered *p*-terphenyl crystal 225 (1994) 116
Bässler, H., see M. Scheidler 225 (1994) 431
Bates, S. and J. Dwyer, Improvements in ab initio calculated OH stretching frequencies of zeolite acid site models and other OH-containing molecules, using a Morse potential 225 (1994) 427
Bauschlicher Jr., C.W., see J.A. Sheehy 225 (1994) 221
Bauschlicher Jr., C.W., see P. Maitre 225 (1994) 467
Bishop, A.R., see S.P. Love 225 (1994) 170
Bondarev, S.L. and V.N. Knyukshto, Fluorescence from the $S_1(2^1A_g)$ state of all-trans-β-carotene 225 (1994) 346
Bondybey, V.E., see J. Agreiter 225 (1994) 87
Botschwina, P., Large-scale ab initio calculations of spectroscopic constants for CNCN 225 (1994) 480
Bräuchle, C., see Th. Basché 225 (1994) 116
Braun, D., A. Ceulemans, B. Dick and H. Konami, Spectral hole burning on silicon phthalocyanines isolated in an argon matrix 225 (1994) 398
Brousseau, J.-L., see C. Garrigou-Lagrange 225 (1994) 297
Brouwer, A.M., F.W. Langkilde, K. Bajdor and R. Wilbrandt, Through-bond interaction in the radical cation of N,N-dimethylpiperazine. Resonance Raman spectroscopy and quantum chemical calculations 225 (1994) 386
Broyer, M., see Ph. Dugourd 225 (1994) 28
Bürgi, T., T. Droz and S. Leutwyler, Ground-state binding energy and vibrations of the carbazole·Ar van der Waals complex by pump/dump-R2PI measurements 225 (1994) 351

Casero-Junquera, E., R. Lawruszczuk, J. Rostas and G. Taieb, Resonance-enhanced two-photon excitation of CaI 225 (1994) 76
Ceulemans, A., see D. Braun 225 (1994) 398
Chabalowski, C.F., see P.J. Stephens 225 (1994) 247
Chandler, G.S., B.N. Figgis, P.A. Reynolds and S.K. Wolff, Ab initio theoretical calculation of experimental structure factors for $(ND_4)_2Cu(SO_4)_2 \cdot 6D_2O$ at 9 K 225 (1994) 421
Chevaleyre, J., see Ph. Dugourd 225 (1994) 28
Chu, S.-I, see Y. Huang 225 (1994) 46
Cleve, B., see M. Scheidler 225 (1994) 431
Colombo, L., see S. Serra 225 (1994) 191
Coppa, N.V., see S.P. Love 225 (1994) 170
Cummins, P.L. and J.E. Gready, The electrostatic potential in the semiempirical molecular orbital approximation 225 (1994) 11
Czuchaj, E., F. Rebentrost, H. Stoll and H. Preuss, Adiabatic potential curves for the Cd_2 dimer 225 (1994) 233

D'Angelo, P., see A. Filipponi 225 (1994) 150
Danovich, D., see U. Samuni 225 (1994) 391
Darwish, A.D., see I.W. Locke 225 (1994) 186
Davidson, M.M. and I.H. Hillier, Calculation of transition state structures and kinetic isotope effects in the Claisen rearrangement of allyl vinyl ether and chorismic acid 225 (1994) 293
Delhaès, P., see C. Garrigou-Lagrange 225 (1994) 297
Devlin, F.J., see P.J. Stephens 225 (1994) 247
Di Cicco, A., see A. Filipponi 225 (1994) 150
Dick, B., see D. Braun 225 (1994) 398
Diemann, E., see A. Müller 225 (1994) 359
Di Maio, F.P., see E. Sicilia 225 (1994) 208
Doraiswamy, S., see M. Roy 225 (1994) 181
Droz, T., see T. Bürgi 225 (1994) 351
Dugourd, Ph., J. Chevaleyre, R. Antoine, M. Broyer, J.P. Wolf and L. Wöste, Isotopic effects in pseudo-rotating homonuclear triatomic molecules. Application to Li_3 225 (1994) 28
Dwyer, J., see S. Bates 225 (1994) 427

Ebata, T., see A. Fujii 225 (1994) 104
Ebbesen, T.W., see M. Kosaka 225 (1994) 161
Eisenegger, J., see M. Tomaselli 225 (1994) 131
Epifanov, S.Yu. and A.A. Vigasin, Contribution of bound, metastable and free states of bimolecular complexes to collision-induced intensity of absorption 225 (1994) 537
Ernst, R.R., see M. Tomaselli 225 (1994) 131

Figgis, B.N., see G.S. Chandler 225 (1994) 421
Filipponi, A., P. D'Angelo, N.V. Pavel and A. Di Cicco, Triplet correlations in the hydration shell of aquaions 225 (1994) 150
Fraenkel, R., see U. Samuni 225 (1994) 391
Fujii, A., T. Sawamura, S. Tanabe, T. Ebata and N. Mikami, Infrared dissociation spectroscopy of the OH stretching vibration of phenol–rare gas van der Waals cluster ions 225 (1994) 104

Garrigou-Lagrange, C., P. Delhaès, V.M. Yartsev, J.-L. Brousseau and R.M. Leblanc, Inelastic electron tunneling spectroscopy of bis(ethylenedithio)tetrathiafulvalene (BEDT-TTF) compounds 225 (1994) 297
Goldberg, N., M. Iraqi, W. Koch and H. Schwarz, Gas-phase characterization of the neutral and cationic Si_2O_2 molecules. A combined experimental and ab initio study 225 (1994) 404
Gowda, D.C., see D.W. Urry 225 (1994) 97
Gready, J.E., see P.L. Cummins 225 (1994) 11
Gruyters, M. and K. Jacobi, Vibrational and rotational modes of physisorbed H_2 and N_2 on Ag(111) surfaces 225 (1994) 309

Haas, Y., see U. Samuni 225 (1994) 391
Hara, K., N. Kometani and O. Kajimoto, Picosecond kinetics of the excited state of 4-(N,N-dimethylamino)triphenylphosphine at high pressures 225 (1994) 381
Harris, K.D.M., see E.J. MacLean 225 (1994) 273
Harris, R.D., see D.W. Urry 225 (1994) 97
Härtle, M., see J. Agreiter 225 (1994) 87
Hecht, L. and L.D. Barron, Linear polarization Raman optical activity. The importance of the non-resonant term in the Kramers–Heisenberg–Dirac dispersion formula under resonance conditions 225 (1994) 519
Hecht, L. and L.D. Barron, Rayleigh and Raman optical activity from chiral surfaces 225 (1994) 525
Hill, W., see B. Wehling 225 (1994) 67
Hillier, I.H., see M.M. Davidson 225 (1994) 293
Hirao, K., see S. Yamanaka 225 (1994) 213
Hiura, H., see M. Kosaka 225 (1994) 161
Hoffman, D.K., see Y. Huang 225 (1994) 37
Hormes, J., see A. Müller 225 (1994) 359
Hrušák, J., D. Schröder and H. Schwarz, Theoretical prediction of the structure and the bond energy of the gold (I) complex $Au^+(H_2O)$ 225 (1994) 416
Huang, Y., D.J. Kouri and D.K. Hoffman, A general, energy-separable polynomial representation of the time-independent full Green operator with application to time-independent wavepacket forms of Schrödinger and Lippmann–Schwinger equations 225 (1994) 37
Huang, Y. and S.-I Chu, A stationary treatment of time-dependent Hamiltonian by the many-mode floquet formalism and its application to the study of effects of laser pulses in multiphoton processes 225 (1994) 46
Hukao, K., see I. Miyagawa 225 (1994) 364
Hurley, M.D., see T.E. Møgelberg 225 (1994) 375

Iraqi, M., see N. Goldberg 225 (1994) 404
Ishii, N. and T. Shimizu, Density-functional-theory calculations of isotropic hyperfine coupling constants of radicals 225 (1994) 462
Itaya, A., see H. Miyasaka 225 (1994) 315

Jackson, K., see E. Kaxiras 225 (1994) 448
Jacobi, K., see M. Gruyters 225 (1994) 309
Jalkanen, K.J., see P.J. Stephens 225 (1994) 247
Janczak, J., R. Kubiak, A. Zaleski and J. Olejniczak, Metallic conductivity and phase transition in Tl_2Pc 225 (1994) 72

Jayaraman, V.K., see S.S. Tambe 225 (1994) 303
Jeevarajan, A.S., M. Khaled and L.D. Kispert, Simultaneous electrochemical and electron paramagnetic resonance studies of keto and hydroxy carotenoids 225 (1994) 340

Kahana, S., see U. Samuni 225 (1994) 391
Kajimoto, O., see K. Hara 225 (1994) 381
Kaluža, M., J.T. Muckerman and H. Rabitz, The role of laser-pulse phases in the sub-picosecond optimal infrared multiphoton dissociation of HF 225 (1994) 335
Kaxiras, E., K. Jackson and M.R. Pederson, Theoretical study of passivated small fullerenes $C_{24}X_4$ (X=N, P, As) and their isoelectronic equivalents $(BN)_{12}X_4$ 225 (1994) 448
Khaled, M., see A.S. Jeevarajan 225 (1994) 340
Kierzkowski, P., R. Ławruszczuk and A. Kowalski, Chemiluminescence of alkaline earth monoiodides in collisions of metastable Mg, Ca and Sr atoms with I_2 225 (1994) 369
Kispert, L.D., see A.S. Jeevarajan 225 (1994) 340
Klockow, D., see B. Wehling 225 (1994) 67
Knyukshto, V.N., see S.L. Bondarev 225 (1994) 346
Koch, W., see N. Goldberg 225 (1994) 404
Kometani, N., see K. Hara 225 (1994) 381
Konami, H., see D. Braun 225 (1994) 398
Kosaka, M., T.W. Ebbesen, H. Hiura and K. Tanigaki, Electron spin resonance of carbon nanotubes 225 (1994) 161
Kotani, S., see H. Miyasaka 225 (1994) 315
Kouri, D.J., see Y. Huang 225 (1994) 37
Kowalski, A., see P. Kierzkowski 225 (1994) 369
Kroto, H.W., see I.W. Locke 225 (1994) 186
Kubiak, R., see J. Janczak 225 (1994) 72
Kuetgens, U., see A. Müller 225 (1994) 359
Kühn, O. and V. May, Dissipative dynamics in a curve-crossing system. The N_2 molecule 225 (1994) 511
Kulkarni, B.D., see S.S. Tambe 225 (1994) 303
Kummer, S., see Th. Basché 225 (1994) 116

Laidig, K.E., Density functional methods and the spatial distribution of electronic charge 225 (1994) 285
Langhoff, S.R., see J.A. Sheehy 225 (1994) 221
Langkilde, F.W., see A.M. Brouwer 225 (1994) 386
Lawruszczuk, R., see E. Casero-Junquera 225 (1994) 76
Ławruszczuk, R., see P. Kierzkowski 225 (1994) 369
Leblanc, R.M., see C. Garrigou-Lagrange 225 (1994) 297
Leutwyler, S., see T. Bürgi 225 (1994) 351
Levine, R.D., see F. Remacle 225 (1994) 503
Li (, F., see L. Xu 225 (1994) 547
Lim, E.C., see R.G. Sadygov 225 (1994) 441
Locke, I.W., A.D. Darwish, H.W. Kroto, K. Prassides, R. Taylor and D.R.M. Walton, Phosphorus/buckminsterfullerene intercalation compound, $C_{60}(P_4)_2$ 225 (1994) 186
Love, S.P., D. McBranch, M.I. Salkola, N.V. Coppa, J.M. Robinson, B.I. Swanson and A.R. Bishop, Near-infrared Raman spectroscopy of solid C_{60}. Raman activation of silent modes by ^{13}C and sample disorder 225 (1994) 170

MacLean, E.J., K.D.M. Harris and S.L. Price, Structural and dynamic properties of hydrogen bonding in a tetrahedral arrangement of methanol molecules. A theoretical investigation 225 (1994) 273
Magyarfalvi, G. and P. Pulay, Basis set and correlation effects in the calculation of selenium NMR shieldings 225 (1994) 280
Maitre, P. and C.W. Bauschlicher Jr., Theoretical study of the low-lying states of MgN_2^+ 225 (1994) 467
Marinelli, F. and M. Roche, Effect of Mg–Mg pairs on the low-temperature lattice specific heat of Al–Mg alloys 225 (1994) 542
Martin, J.M.L. and P.R. Taylor, Basis set convergence for geometry and harmonic frequencies. Are h functions enough? 225 (1994) 473
Martínez, J.M., see R.R. Pappalardo 225 (1994) 202
Marumo, S., see A. Osuka 225 (1994) 140
Maruyama, K., see A. Osuka 225 (1994) 140
Mataga, N., see A. Osuka 225 (1994) 140
May, V., see O. Kühn 225 (1994) 511
McBranch, D., see S.P. Love 225 (1994) 170
Meier, B.H., see M. Tomaselli 225 (1994) 131
Meyer, W., see J. Stärck 225 (1994) 229
Mikami, N., see A. Fujii 225 (1994) 104
Miyagawa, I., K. Sogabe, M. Ohuchi and K. Hukao, Study of an activated carbon by the ESR triple-modulation spectrum method 225 (1994) 364
Miyasaka, H., T. Moriyama, S. Kotani, R. Muneyasu and A. Itaya, Picosecond dynamics of photoinduced electron transfer processes in poly(N-vinylcarbazole) solid film doped with electron acceptors as revealed by transient absorption spectroscopy and dichroism measurements 225 (1994) 315
Möbius, D., see L. Wolthaus 225 (1994) 322
Møgelberg, T.E., O.J. Nielsen, J. Sehested, T.J. Wallington, M.D. Hurley and W.F. Schneider, Atmospheric chemistry of HFC-134a. Kinetic and mechanistic study of the $CF_3CFHO_2 + NO_2$ reaction 225 (1994) 375
Morikami, K. and M. Saito, Molecular dynamics study on the stability of ions around human lysozyme in the crystal condition 225 (1994) 196
Moriyama, T., see H. Miyasaka 225 (1994) 315
Muckerman, J.T., see M. Kaluža 225 (1994) 335
Müller, A., V. Wittneben, E. Diemann, J. Hormes and U. Kuetgens, Electronic structure of thiometalates $[MS_4]^{n-}$ (M = Mo, W, Re). XANES spectra and SCF-Xα-SW calculations 225 (1994) 359
Muneyasu, R., see H. Miyasaka 225 (1994) 315
Murad, S. and J.G. Powles, Computer simulation of osmosis and reverse osmosis in solutions 225 (1994) 437

Nielsen, O.J., see T.E. Møgelberg 225 (1994) 375
Nishimura, Y., see A. Osuka 225 (1994) 140
Novoa, J.J., M. Planas and M.-H. Whangbo, A numerical evaluation of the counterpoise method on hydrogen bond complexes using near complete basis sets 225 (1994) 240

Ohkohchi, M., see A. Osuka 225 (1994) 140
Ohuchi, M., see I. Miyagawa 225 (1994) 364
Okada, T., see A. Osuka 225 (1994) 140
Okumura, M., see S. Yamanaka 225 (1994) 213

Olejniczak, J., see J. Janczak 225 (1994) 72
Osuka, A., S. Marumo, K. Maruyama, N. Mataga, M. Ohkohchi, S. Taniguchi, T. Okada, I. Yamazaki and Y. Nishimura, Picosecond excited-state dynamics of fixed-distance triads consisting of metalloporphyrin, doubly strapped metal-free porphyrin, and pyromellitimide 225 (1994) 140
Oyler, N.A., see G.H. Roehrig 225 (1994) 265

Pappalardo, R.R., J.M. Martínez and E. Sánchez Marcos, Geometrical structure of the cis- and trans-isomers of 1,2-dihaloethylenes and the energetics of their chemical equilibrium in solution 225 (1994) 202
Park, H. and R.N. Zare, Evidence for a Cooper minimum in the photoionization dynamics of the NO D $^2\Sigma^+$ state 225 (1994) 327
Parker, T.M., see D.W. Urry 225 (1994) 97
Partridge, H., see J.A. Sheehy 225 (1994) 221
Pavel, N.V., see A. Filipponi 225 (1994) 150
Pederson, M.R., see E. Kaxiras 225 (1994) 448
Peng, S., see D.W. Urry 225 (1994) 97
Pick, Š., Tight-binding model of hydrogen chemisorption on Pd/Ta (110) and Pd/W (110) surfaces 225 (1994) 62
Planas, M., see J.J. Novoa 225 (1994) 240
Powles, J.G., see S. Murad 225 (1994) 437
Prassides, K., see I.W. Locke 225 (1994) 186
Preuss, H., see E. Czuchaj 225 (1994) 233
Price, S.L., see E.J. MacLean 225 (1994) 273
Pulay, P., see G. Magyarfalvi 225 (1994) 280

Rabitz, H., see M. Kaluža 225 (1994) 335
Rebentrost, F., see E. Czuchaj 225 (1994) 233
Remacle, F. and R.D. Levine, Interference effects in product state distributions using time domain information 225 (1994) 503
Reynolds, P.A., see G.S. Chandler 225 (1994) 421
Rice, S.A., see B. Amstrup 225 (1994) 1
Riera, A., Application of the multi-channel Landau–Zener model to stabilization graphs 225 (1994) 531
Robinson, J.M., see S.P. Love 225 (1994) 170
Roche, M., see F. Marinelli 225 (1994) 542
Roehrig, G.H., N.A. Oyler and L. Adamowicz, Can electron attachment alter tautomeric equilibrium of guanine? Theoretical ab initio study 225 (1994) 265
Rostas, J., see E. Casero-Junquera 225 (1994) 76
Roy, M. and S. Doraiswamy, Rotational dynamics of C_{60} and C_{70}. Investigation by picosecond fluorescence time-resolved anisotropy decay 225 (1994) 181
Russo, N., see E. Sicilia 225 (1994) 208

Sadygov, R.G. and E.C. Lim, A theoretical study of the structure and energetics of stacked dimers of polycyclic aromatic hydrocarbons. Application of INDO 1/S method to singlet excimers of naphthalene and phenanthrene 225 (1994) 441
Saito, M., see K. Morikami 225 (1994) 196
Salkola, M.I., see S.P. Love 225 (1994) 170

Samuni, U., S. Kahana, R. Fraenkel, Y. Haas, D. Danovich and S. Shaik, The ICN–INC system: experiment and quantum chemical calculations 225 (1994) 391
Sánchez Marcos, E., see R.R. Pappalardo 225 (1994) 202
Sanctuary, B.C., see S.Z. Ageev 225 (1994) 499
Sanguinetti, S., see S. Serra 225 (1994) 191
Satpathy, S., see M. Springborg 225 (1994) 454
Sawamura, T., see A. Fujii 225 (1994) 104
Schaper, A., see L. Wolthaus 225 (1994) 322
Scheidler, M., B. Cleve, H. Bässler and P. Thomas, Monte Carlo simulation of bimolecular exciton annihilation in an energetically random hopping system 225 (1994) 431
Schlegel, H.B., see P.Y. Ayala 225 (1994) 410
Schneider, W.F., see T.E. Møgelberg 225 (1994) 375
Schröder, D., see J. Hrušák 225 (1994) 416
Schwarz, H., see N. Goldberg 225 (1994) 404
Schwarz, H., see J. Hrušák 225 (1994) 416
Sehested, J., see T.E. Møgelberg 225 (1994) 375
Sekino, H. and R.J. Bartlett, Nuclear coupling constants obtained by the equation-of-motion coupled cluster theory 225 (1994) 486
Serra, S., S. Sanguinetti and L. Colombo, Pre-fragmentation dynamics of C_{60}. A molecular dynamics investigation 225 (1994) 191
Shaik, S., see U. Samuni 225 (1994) 391
Sheehy, J.A., C.W. Bauschlicher Jr., S.R. Langhoff and H. Partridge, Theoretical study of the nitric oxide ϵ and 11000 Å bands 225 (1994) 221
Shimizu, T., see N. Ishii 225 (1994) 462
Sicilia, E., F.P. Di Maio and N. Russo, Features of the potential energy surface for the CH_3+O_2 reaction channels 225 (1994) 208
Siddles, R.M., G.J. Wilson and C.J.S.M. Simpson, The vibrational deactivation of the (00^01) mode of N_2O measured down to 150 K 225 (1994) 146
Simpson, C.J.S.M., see R.M. Siddles 225 (1994) 146
Smith, A.M., see J. Agreiter 225 (1994) 87
Sogabe, K., see I. Miyagawa 225 (1994) 364
Springborg, M. and S. Satpathy, Density-functional calculations of electronic and structural properties of small fullerene tubules 225 (1994) 454
Stärck, J. and W. Meyer, Long-range interaction potential of the $^5\Sigma_g^+$ state of He_2 225 (1994) 229
Stephens, P.J., C.F. Chabalowski, F.J. Devlin and K.J. Jalkanen, Ab initio calculation of vibrational circular dichroism spectra using large basis set MP2 force fields 225 (1994) 247
Stoll, H., see E. Czuchaj 225 (1994) 233
Stratton, J.R., T. Troxler and M.R. Topp, Structural measurements of perylene clusters with cyclopropane via rotational coherence spectroscopy 225 (1994) 108
Stuchebrukhov, A.A., Dispersion relations for electron and hole transfer in donor–bridge–acceptor systems 225 (1994) 55
Surján, P. and J.G. Ángyán, The reliability of the point charge model representing intermolecular effects in ab initio calculations 225 (1994) 258
Swanson, B.I., see S.P. Love 225 (1994) 170

Taieb, G., see E. Casero-Junquera 225 (1994) 76
Tambe, S.S., V.K. Jayaraman and B.D. Kulkarni, Cellular automata modelling of a surface catalytic reaction with Eley–Rideal step: the case of CO oxidation 225 (1994) 303

Tanabe, S., see A. Fujii 225 (1994) 104
Tanigaki, K., see M. Kosaka 225 (1994) 161
Taniguchi, S., see A. Osuka 225 (1994) 140
Taylor, P.R., see J.M.L. Martin 225 (1994) 473
Taylor, R., see I.W. Locke 225 (1994) 186
Teki, Y., J.U. von Schütz, H. Wachtel, V. Weiss and H.C. Wolf, Triplet excitons in diphenylbutadiene and diphenylhexatriene single crystals by zero-field delayed fluorescence ODMR 225 (1994) 124
Thomas, P., see M. Scheidler 225 (1994) 431
Tomaselli, M., B.H. Meier, M. Baldus, J. Eisenegger and R.R. Ernst, An rf-driven nuclear spin-diffusion experiment using zero-angle sample spinning 225 (1994) 131
Topp, M.R., see J.R. Stratton 225 (1994) 108
Troxler, T., see J.R. Stratton 225 (1994) 108

Urry, D.W., S. Peng, D.C. Gowda, T.M. Parker and R.D. Harris, Comparison of electrostatic- and hydrophobic-induced pK_a shifts in polypentapeptides. The lysine residue 225 (1994) 97

Varandas, A.J.C., A novel non-active model to account for the leak of zero-point energy in trajectory calculations. Application to $H+O_2$ reaction near threshold 225 (1994) 18
Vigasin, A.A., see S.Yu. Epifanov 225 (1994) 537
Von Schütz, J.U., see Y. Teki 225 (1994) 124

Wachtel, H., see Y. Teki 225 (1994) 124
Wallington, T.J., see T.E. Møgelberg 225 (1994) 375
Walton, D.R.M., see I.W. Locke 225 (1994) 186
Wang, P., see L. Xu 225 (1994) 547
Wang, S. and D. Zhou, Microscopy of single-layer carbon nanotubes 225 (1994) 165
Wang, Y., see L. Xu 225 (1994) 547
Wehling, B., W. Hill and D. Klockow, Crosslinking of organic acid and isocyanate to silver SERS substrates by mercaptoethanol 225 (1994) 67
Weiss, V., see Y. Teki 225 (1994) 124
Whangbo, M.-H., see J.J. Novoa 225 (1994) 240
Wilbrandt, R., see A.M. Brouwer 225 (1994) 386
Wilson, G.J., see R.M. Siddles 225 (1994) 146
Wittneben, V., see A. Müller 225 (1994) 359
Wolf, H.C., see Y. Teki 225 (1994) 124
Wolf, J.P., see Ph. Dugourd 225 (1994) 28
Wolff, S.K., see G.S. Chandler 225 (1994) 421
Wolthaus, L., A. Schaper and D. Möbius, Brickstone arrangement in J-aggregates of an amphiphilic merocyanine dye 225 (1994) 322
Wöste, L., see Ph. Dugourd 225 (1994) 28

Xu, L., Y. Wang, P. Wang and F. Li, High-resolution (2+1) multiphoton ionization spectroscopy of Br_2 (Chem. Phys. Letters 212 (1993) 265). Erratum 225 (1994) 547

Yamaguchi, K., see S. Yamanaka 225 (1994) 213
Yamanaka, S., M. Okumura, K. Yamaguchi and K. Hirao, CASPT2 and MR MP2 calculations of potential curves and effective exchange integrals for the dimer of triplet methylene 225 (1994) 213

Yamazaki, I., see A. Osuka 225 (1994) 140
Yartsev, V.M., see C. Garrigou-Lagrange 225 (1994) 297
Yoshimori, A., Symmetry of a free energy curve in polar solution 225 (1994) 494

Zaleski, A., see J. Janczak 225 (1994) 72
Zare, R.N., see H. Park 225 (1994) 327
Zhou, D., see S. Wang 225 (1994) 165